Transitional Flow Parameter Based on Entropy Generation

Multi-Algorithm Methods for Multi-Scale Simulations
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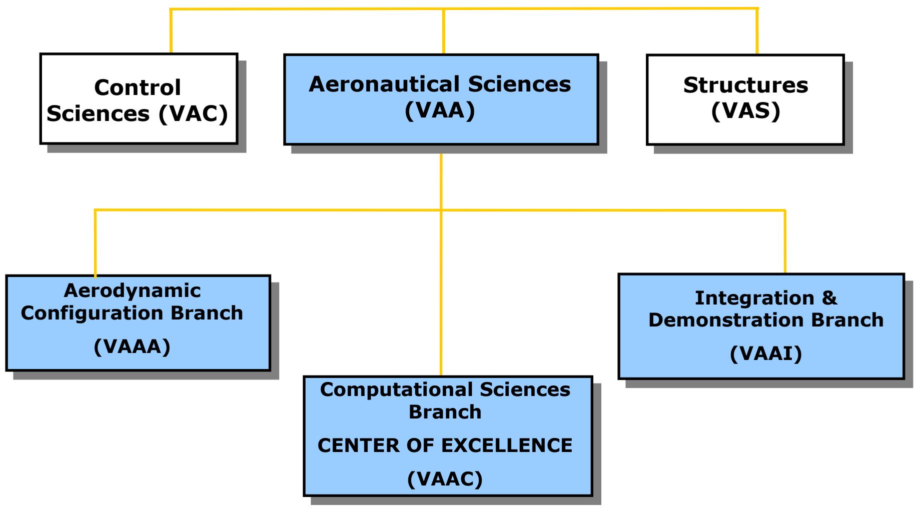
Objective & Motivation

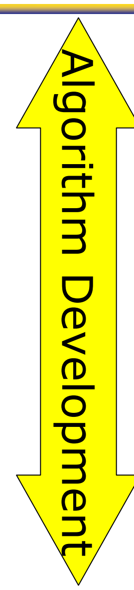
- **Objective**
  - To introduce the idea of using entropy-based criteria for the analyzing the onset of significant non-equilibrium effects which invalidate the governing equations of CFD.
- **Motivation**
  - Continuum fluid flow solvers well-understood; modeling and simulation capabilities well-developed.
  - Rarefied gas dynamics well-understood; modeling and simulation capabilities well-developed.
  - Under extreme environments, overlapping regions appear where continuum assumption no longer holds but full molecular simulation still inefficient.

Air Vehicles Directorate Technical Divisions



Current Emphasis

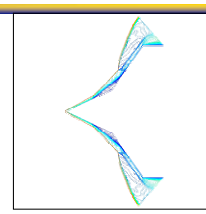
- **Multidisciplinary Computational Sciences**
  - Fluid-Structure Interaction; Acoustics.
  - Turbulence Modeling and Simulation, DNS/LES.
- **Electromagnetics**
  - Radar-Cross Section Prediction
  - Antenna Analysis & Design
- **Hypersonics; Plasma Dynamics**
  - Magneto-Aerodynamics
  - Chemical & Thermal Non-Equilibrium
- **Computational Aerodynamics**
  - Full-Scale Vehicle Flow Simulations
  - Unstructured RANS



Computational Aerothermodynamics
NATO RTO / AFOSR Validation Cases

M = 9.49
Re_L=1.28 x 10^4
25/55 degree cone
Axisymmetric Laminar Flow
CUBRC Data (Mike Holden)

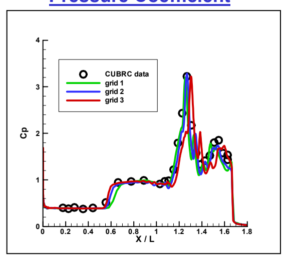
Mach Contours



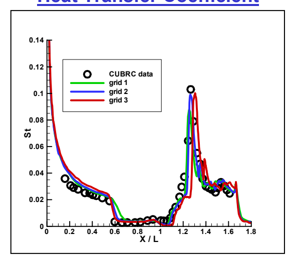
Baseline $Cobalt_{60}$ Results

PoC: Dr. Jim Miller
AFRL/VAAC

Pressure Coefficient



Heat Transfer Coefficient



Validation Studies for High Mach Number Flows

Unified Approach for Continuum to Rarefied Flow

PoC: Eswar Josyula
AFRL/VAAC

- **Objective**
  - Develop a unified computational code to simulate gas flows in rarefied and continuum regimes
- **Product**
  - A single computational code to treat hypersonic re-entry flows across the rarefied and continuum flight regimes
- **Metrics**
  - Demonstrate ability to solve hypersonic re-entry flow past a blunt body for Knudsen numbers of 0.001 to 1 to achieve (a) converged solutions, (b) efficient solutions based on corresponding CFD and DSMC solutions, (c) accurate solutions corresponding to the CFD and DSMC solutions

Basic Aspects of High-T Flow

- **Thermodynamic properties ($e, h, p, T, \rho, s,\ldots$)**
- **Transport properties ($\mu, \kappa, D_{i,j}$) → $f(T,p)$**
- **High heating rates dominant aspect.**
- **Ratio of specific heats no longer constant.**
- **Possible ionization; gas mixture → partially ionized plasma.**
- **Possible effects of radiation to/from gas mixture/plasma.**
- ***Virtually all analyses of high-temperature flows require numerical solution.***

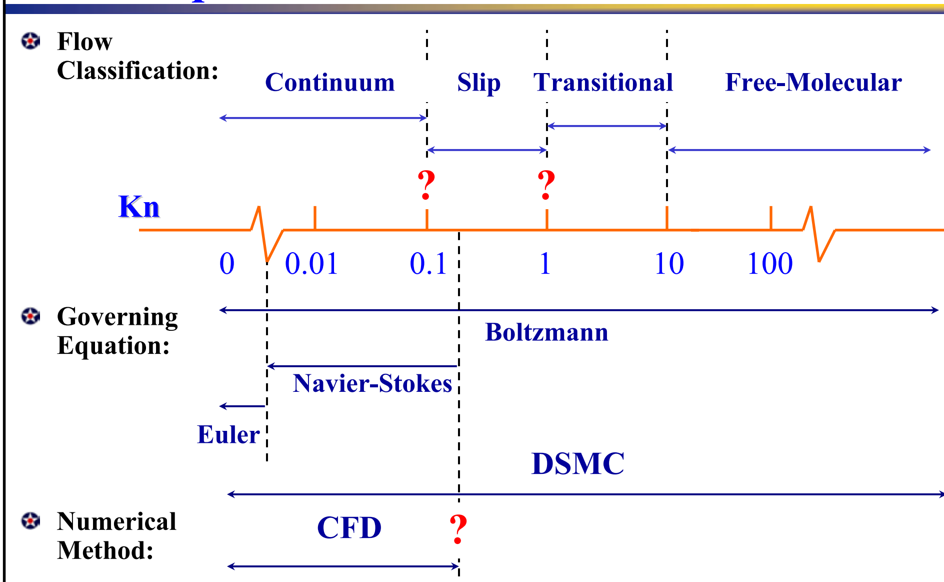
Transport Properties

- **Gradients in the physical properties (velocity, temperature, species concentration, etc) induce molecular transport which is directly proportional to the gradient but in the opposite direction.**
  - Viscosity, heat conduction, mass diffusion.
- **Coefficients of viscosity, thermal conductivity, and diffusion → Transport Properties.**

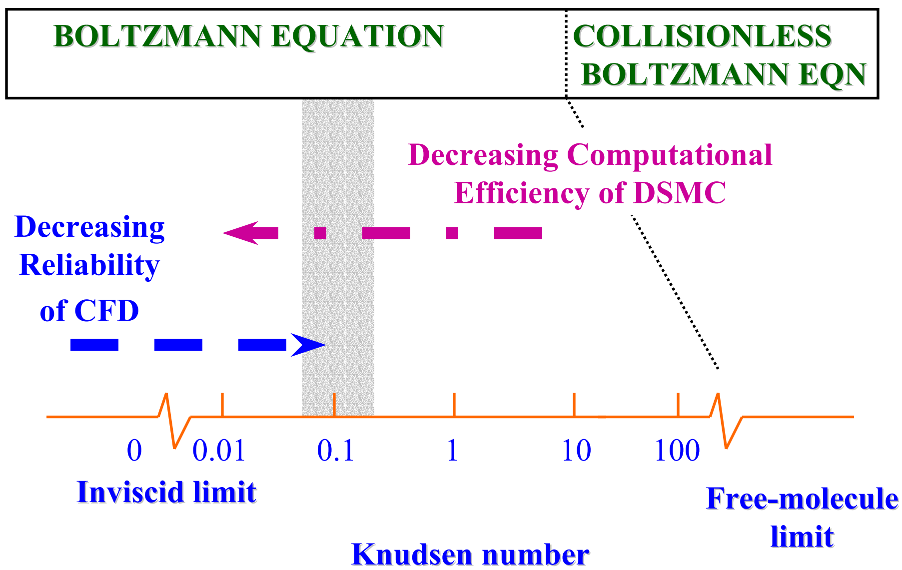
Conceptual Details

- **Fluid Mechanics.**
  - Physics: Conservation of Mass, Momentum, and Energy.
  - Local Thermodynamic Equilibrium.
  - Continuum ←→ Field Variables.
- **What does “continuum breakdown” mean?**
  - Assumption in deriving equations no longer holds.
  - May be brought on by:
    - Rarefied gas flow (low density) → insufficient molecules for meaningful statistics.
    - Extreme gradients in macroscopic variables → transport models (constitutive equations) no longer valid.
    - Micro-scale gas flows (length scale of interest approaches molecular mean-free path).

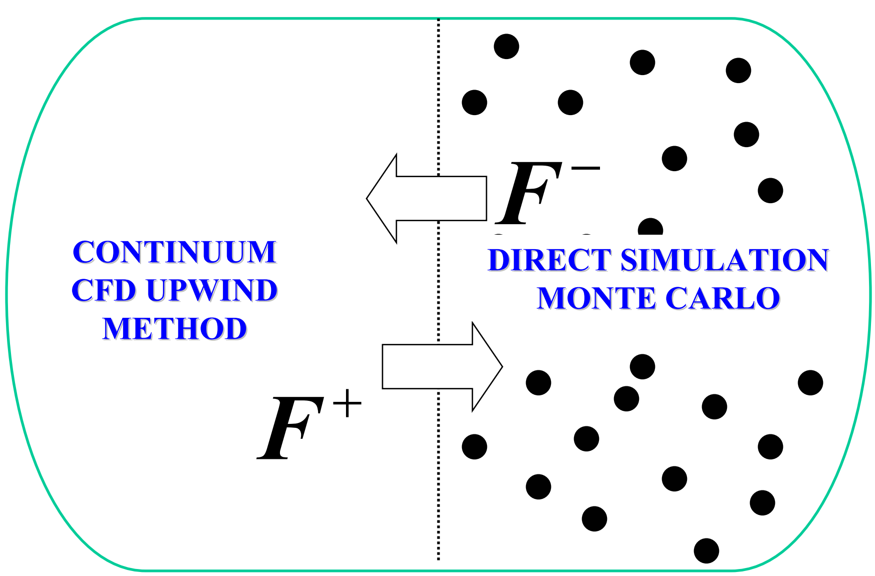
Flow Regimes, Mathematical Equations, and Numerical Solvers



Rationale for Hybrid Coupling



Schematic of Cell Interface



Hybrid Numerical Method: Coupling CFD and DSMC

- **Primary Challenges**
  - When to use one method or the other.
  - How to pass information at interface between methods.
  - Combined algorithm for efficient vector and parallel processing.
- **Switching Criteria**
  - Assume: DSMC "solves" Boltzmann equation.
  - Boltzmann equation applies across Knudsen number regime.
  - Therefore, DSMC solutions reliably accurate.
  - To decide when continuum breakdown occurs, compare CFD solutions to DSMC under conditions expected to challenge CFD (Navier-Stokes) accuracy.

Breakdown Criteria

- **Breakdown Criteria**
  - Need a reliable, robust, easy-to-calculate parameter that signals the onset of non-equilibrium beyond the modeling capability of the Navier-Stokes Equations.
  - Compare CFD to DSMC solutions and decide how much difference is acceptable (5%? 10%?).
  - Check value of parameter when the difference in solution is beyond acceptable range.
  - Reliable parameter will exceed a consistent value in a variety of flow conditions signaling unacceptable difference between CFD and DSMC solutions.

CFD to DSMC Switching Criteria

- **Knudsen**

$$Kn = \frac{\lambda}{L} > 0.10$$

$$L = \begin{cases} \text{Global Body Length} \\ \text{Local Gradient Length} \end{cases}$$

$$\lambda = \begin{cases} \text{Freestream} \\ \text{Local MFP} \end{cases}$$

- **G. Bird**
  - (1970) *AIAA Journal* **8** (11)

$$P = -\frac{1}{\nu_{\text{collisons}}}\left(\frac{D(\ln\rho)}{Dt}\right) = -\sqrt{\frac{\pi\gamma}{8}}M\,\frac{\lambda}{\rho}\frac{d\rho}{dx} > 0.04$$

- **Boyd, et al.**
  - (1995) *Physics of Fluids*, **7** (1)

$$Kn_Q = \frac{\lambda}{Q}\left|\frac{dQ}{dl}\right| > 0.05$$

  - Local Gradient Length-Scale:

$$Kn_Q = \frac{\lambda}{Q}\left|\nabla Q\right| > 0.05$$

Generalized Continuum Breakdown Parameters

- **W. Wang & I. D. Boyd**
  - AIAA Paper 2002-0651, January 2002
  - To accommodate viscous and heating effects, evaluated a variety of parameters with local length-scales based on:
    - Density Kn_D P_D
    - Velocity Kn_V P_V
    - Temperature Kn_T P_T
  - Switching Criteria Based on:

$$Kn_{\max} = \max\left(Kn_D, Kn_V, Kn_T\right)$$
$$P_{\max} = \max\left(P_D, P_V, P_T\right)$$

  - Fractional Difference:

$$\varepsilon_Q = \frac{Q_{CFD} - Q_{DSMC}}{Q_{DSMC}}$$

Common Features

- **P-type Parameters:** $P_Q = \sqrt{\frac{\pi\gamma}{8}} M \frac{\lambda}{Q} |\nabla Q|$
  - Local Gradient-Based length scale.
  - Variable can be density, temperature, velocity, pressure (?).
- **Knudsen-type Parameters:** $Kn_Q = \frac{\lambda}{Q} |\nabla Q|$
  - Local gradient-based length scale.
  - Variable can be density, temperature, velocity, pressure (?).
- **Other Parameters:**
  - P. Canupp (1997, 2000); Garcia, et. al, JCP 1999.

Viscous stress: $K_\tau = \frac{|\tau|}{p}$ Heat Flux: $K_q = \frac{|q|}{pc}$

Abstract Common Elements

- **Why Entropy and the Second Law?**
  - Universality! SLT for any physical process.
- **Entropy generation captures essential features of non-equilibrium.**
- **For NSE:**
  - Quantifies irreversibility associated with velocity and temperature gradients via transport properties.
- **Can it be generalized for higher-order models?**
  - BGK-Burnett?
  - DSMC?

Constitutive Formula for the Entropy Generation Rate

- **Essence of the second law:** $\exists S = S(\boldsymbol{q}) \ni$

$$\boxed{S(\boldsymbol{q}_0) - S(\boldsymbol{q}) - \left.\frac{\partial S}{\partial \boldsymbol{q}}\right|_0 \cdot (\boldsymbol{q}_0 - \boldsymbol{q}) \geq 0}$$

- **Time-rate of change:** $\dfrac{\partial S}{\partial t} - \dfrac{\partial S}{\partial \boldsymbol{q}} \cdot \dfrac{\partial \boldsymbol{q}}{\partial t} = 0$

- **Navier-Stokes Equations:** $\dfrac{\partial \boldsymbol{q}}{\partial t} + \dfrac{\partial \boldsymbol{f}_j}{\partial x_j} + \dfrac{\partial \boldsymbol{f}_j^v}{\partial x_j} = 0$

Entropy Generation Formulas

- **Transport of Entropy Equation**

$$\boxed{\dot{S}^t_{\text{gen}} = \frac{\partial \rho s}{\partial t} + \frac{\partial \rho u_j s}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\frac{q_j}{T}\right)}$$

- **Constitutive Formula:**

$$\boxed{\dot{S}^c_{\text{gen}} = \frac{\tau_{ij}}{T}\frac{\partial u_i}{\partial x_j} - \frac{q_k}{T^2}\frac{\partial T}{\partial x_k}}$$

- **Constitutive Relations**

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \lambda \frac{\partial u_k}{\partial x_k}\delta_{ij} \qquad q_k = -\kappa \frac{\partial T}{\partial x_k}$$

Transitional Flow Parameters Based on Entropy

Transitional Flow Parameters

- Bird (1970)

$$P = -\frac{1}{\nu_{\text{collisons}}}\left(\frac{D(\ln\rho)}{Dt}\right) = -\sqrt{\frac{\pi\gamma}{8}}M\frac{\lambda}{\rho}\frac{d\rho}{dx} > 0.04$$

- Ideal Gas Entropy Formula: $s = f(\rho, T)$

- Entropy Balance: $\frac{\dot{S}^{t}_{\text{gen}} - \nabla\cdot(\vec{q}/T)}{\rho} = \frac{\partial s}{\partial t} + u_j\frac{\partial s}{\partial x_j} = \frac{Ds}{Dt}$

- Entropy-Based Parameter:

$$\boxed{P_S \equiv \frac{1}{\nu_{collisions}}\left|\frac{Ds}{Dt}\right| = \sqrt{\frac{\pi\gamma}{8}}M\lambda\left|\frac{ds}{dx}\right|}$$

Transitional Flow Parameters Based on Entropy-Generation

Transport-Based Parameters:

$$K_\tau = \frac{|\tau|}{p} \qquad K_q = \frac{|q|}{pc}$$

Entropy Generation Rate:

$$\boxed{\dot{S}^{c}_{\text{gen}} = \frac{\tau_{ij}}{T}\frac{\partial u_i}{\partial x_j} - \frac{q_k}{T^2}\frac{\partial T}{\partial x_k}}$$

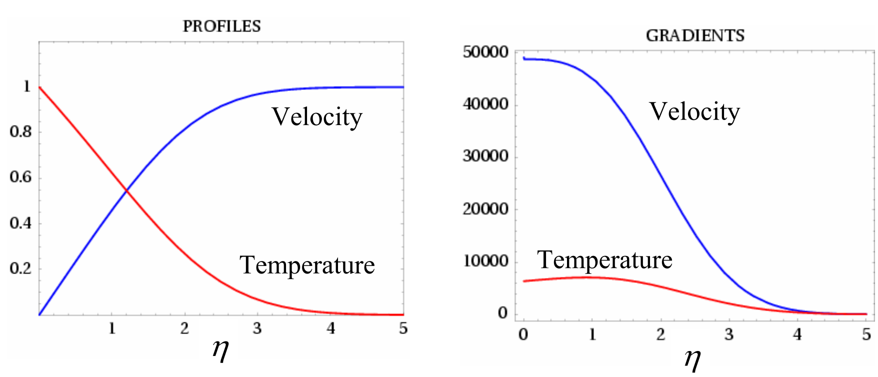
Dimensionless Parameter:

$$\boxed{K_S \equiv \frac{\ell\dot{S}^{c}_{\text{gen}}}{\rho R\sqrt{RT}} = \frac{\lambda}{[P/T]_{\text{REF}}[U]_{\text{REF}}/\dot{S}^{c}_{\text{gen}}}}$$

Comparison of Breakdown Parameters Based on Entropy

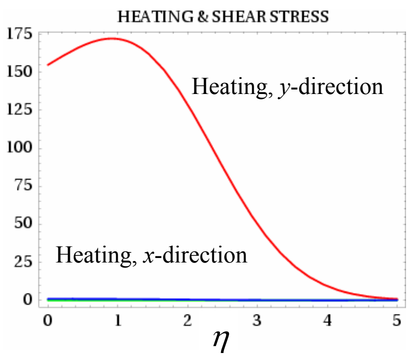
- **Important flow features:**
  - Boundary Layers and Shock Waves.
  - Both exhibit high-gradient profiles.
  - Both are regions where entropy generation may be substantial.
- **Examples:**
  - Boundary layer calculations at M=0.2
    - ODE Blasius equation and energy equations.
  - One-Dimensional Navier Stokes at M=2.0
    - Fully coupled ODEs including viscous stress and heating with Sutherland formulas for transport properties.
  - *Mathematica* used for numerical integration and calculation of results and graphs.

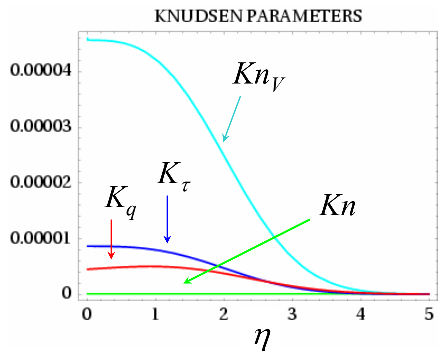
Boundary Layer Profile



- **Velocity boundary layer edge at $\eta \sim 3.5$**
- **Length scale based on plate length of 1.**
- **More severe gradients expected at leading edge.**

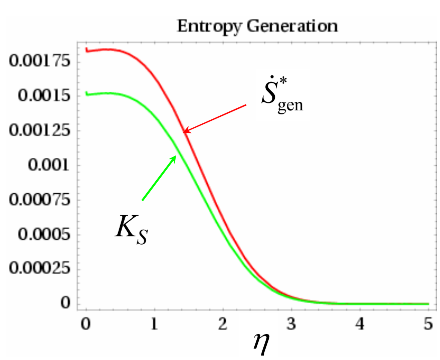
Boundary Layer Calculations

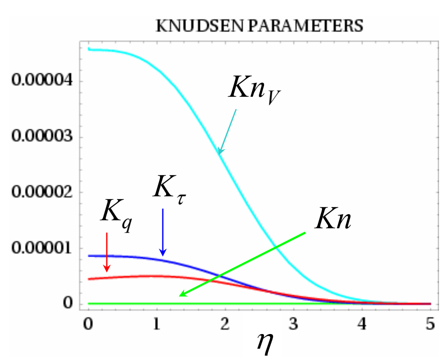




- Heating primarily in direction normal to plate.
- Viscous dissipation very small → low Eckert number approximation valid (typically assumed to simplify energy equation).

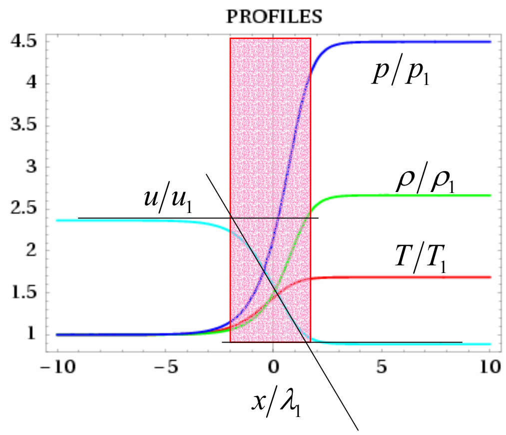
Boundary Layer Calculations





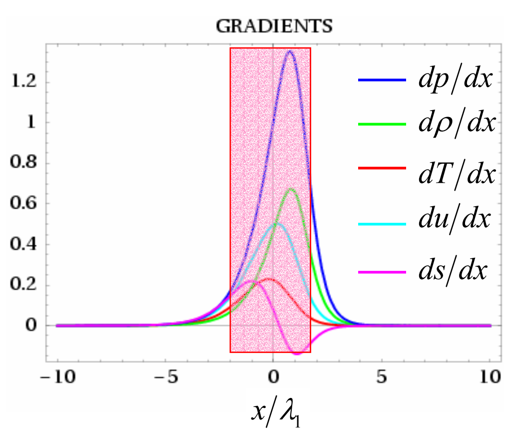
- Entropy generation parameter 2 orders of magnitude larger than others.
- As leading edge approached, would indicate onset of extreme gradients sooner.

Shock Profile: Macroscopic Variables



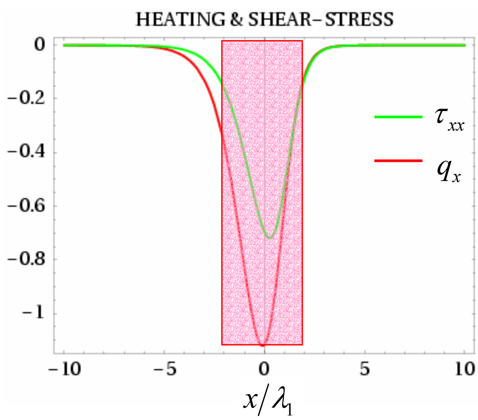
- **Numerical solution of 1D nonlinear Navier-Stokes equations at M=2.0**
  - Fully coupled.
  - Sutherland formula for viscosity and conductivity.
  - Second-law calculations included.

Variable Gradients



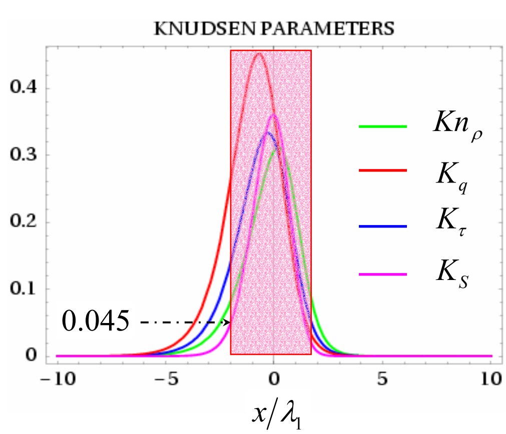
- **Numerical solution of 1D nonlinear Navier-Stokes equations at M=2.0**
  - Pressure gradients largest.
  - Entropy gradients change sign → non-monotonic entropy profile predicted by theory.

Heating and Shear Stress



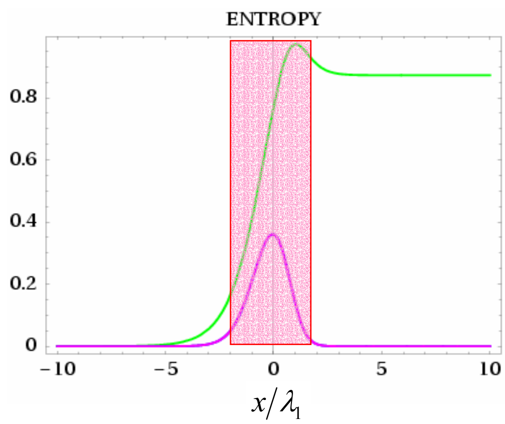
- **Numerical solution of 1D nonlinear Navier-Stokes equations at M=2.0**
  - Peak heating and peak stress almost at the same point.
  - Shock reference location centered at peak entropy generation.

Breakdown Parameters



- **Knudsen-like parameters**
  - Kn → length scale based on mass density gradient.
  - K_τ → based on magnitude of viscous stress.
  - K_q → based on heating.
  - K_S → Entropy generation.
- **Continuum Breakdown**
  - *CBP* ≥ 0.045 at leading edge of shock.
  - *CBP* ≥ 0.01 at trailing edge of shock.
  - Heating seems to indicate breakdown sooner.

Entropy Profile



- **P-type parameters**
  - TBD.
  - Does non-monotonic behavior of entropy profile offer advantage?
- **What value to select for CBP?**
  - 0.10?
  - 0.05?
  - 0.01?
- **Other questions:**
  - Calculate Kn_Q, P_Q with CFD or DSMC?
  - S_{gen} with DSMC?
  - Grid-Based length scale?

Moment Equations

BOLTZMANN EQUATION

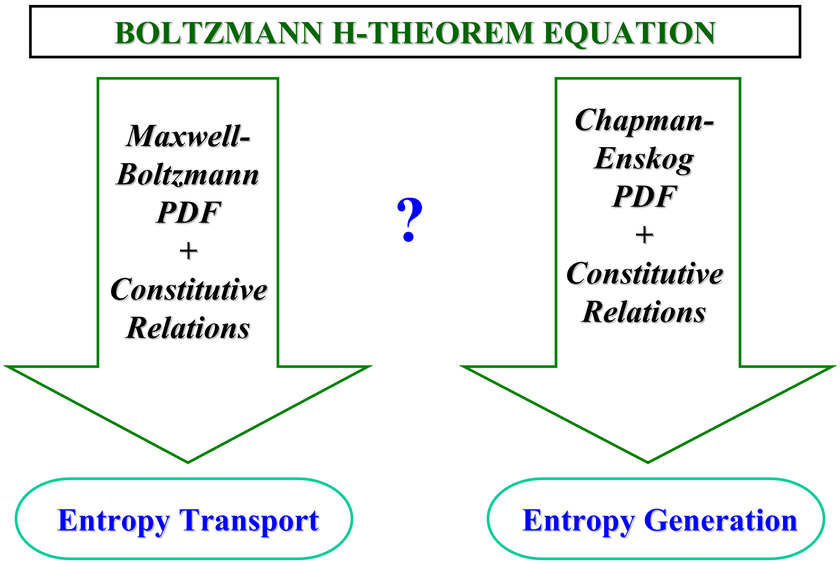
Maxwell-Boltzmann PDF + Constitutive Relations

EULER EQUATIONS

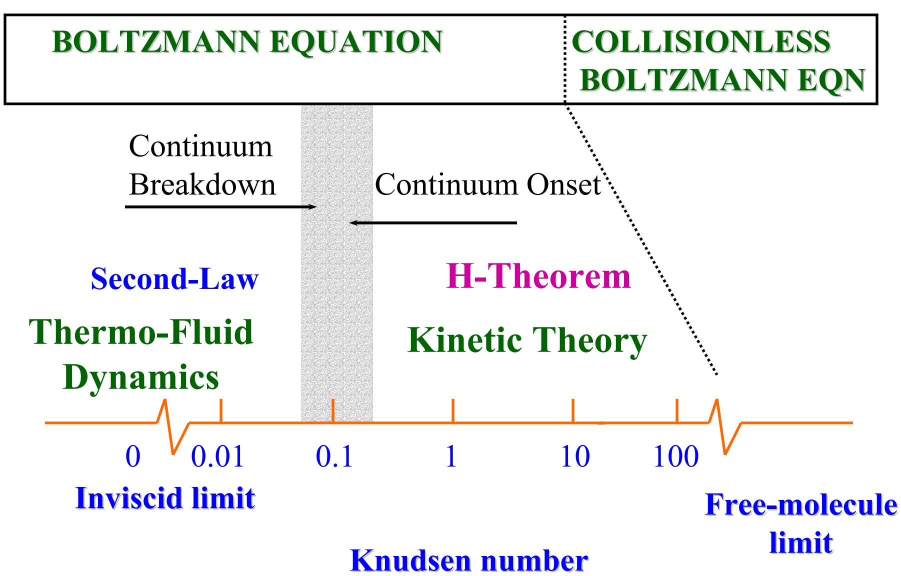
Chapman-Enskog PDF + Constitutive Relations

NAVIER-STOKES

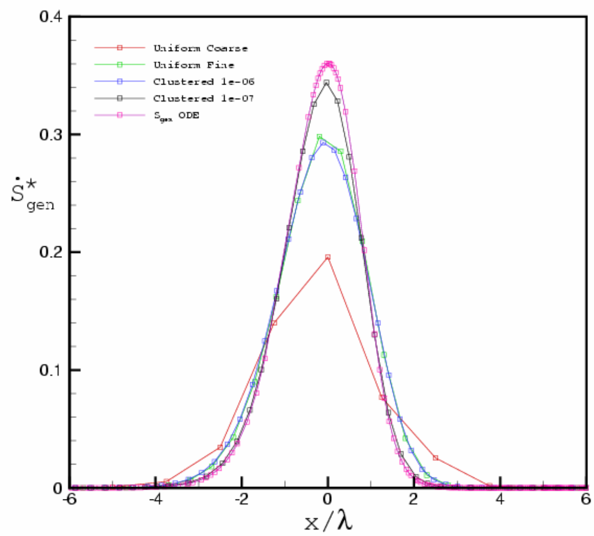
Entropy Moment Equations



Continuum Onset/Breakdown



Entropy Production Comparison



***Cobalt₆₀* CFD Code**

- ☆ Second-order derivatives.
- ☆ Entropy generation formula for viscous, compressible flow.
- ☆ Sutherland formula for viscosity; Eucken relation for conductivity.

S_{gen} → compared with numerical solution of 1D NSE ODEs.

Future Plans

- **Some References:**
  - ☆ AIAA Reno 2002 paper by Wang & Boyd.
  - ☆ AIAA Reno 2003 paper by Camberos & Chen.
  - ☆ AIAA Orlando 2003 paper by Chen/Boyd/Camberos.
- **Short Term:**
  - ☆ Continue collaborative efforts with U. Michigan.
  - ☆ Research proposals for follow-on funding.
- **Some fundamental questions:**
  - ☆ Subtle issues of comparing CFD to DSMC.
  - ☆ Any (simple) flow conditions with analytic solution for baseline comparison?
  - ☆ Asymptotic analysis to better identify transition region?

Closing Remarks

- **The Second Law of Thermodynamics asserts the concavity property of the entropy.**
  - SLT provides criteria for selecting correct, physically relevant solutions generated from mathematical modelling of natural phenomena → *Reliable "Guardian of Reality".*
- **Utility of SLT in CFD/DSMC Coupling Strategies**
  - Continuum breakdown parameter based on entropy and entropy generation compares well with other possibilities.
  - Examples presented entirely within the scope of continuum assumption. Extreme cases analyzed remain inconclusive.
  - Many more questions raised → *To Be Continued!*

Acknowledgements

- **Funding:**
  - AFOSR (Dr. J. Schmisseur, Program Manager)
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  - Iain D. Boyd.
    - DSMC and Hybrid Methods Expert.
    - Department of Aerospace Engineering, University of Michigan.